

# FEM FOR TIME-FRACTIONAL DIFFUSION EQUATIONS, NOVEL OPTIMAL ERROR ANALYSES

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**ABSTRACT.** A semidiscrete Galerkin finite element method applied to time-fractional diffusion equations with time-space dependent diffusivity on bounded convex spatial domains will be studied. The main focus is on achieving optimal error results with respect to both the convergence order of the approximate solution and the regularity of the initial data. By using novel energy arguments, for each fixed time  $t$ , optimal error bounds in the spatial  $L^2$ - and  $H^1$ -norms are derived for both cases: smooth and nonsmooth initial data.

## 1. INTRODUCTION

In this work, we consider the spatial discretisation via Galerkin finite elements of the following time-fractional diffusion problem: find  $u = u(x, t)$  so that

$$(1.1a) \quad {}^C\partial_t^\alpha u(x, t) - \operatorname{div}(\kappa_\alpha(x, t)\nabla u(x, t)) = 0 \quad \text{in } \Omega \times (0, T],$$

$$(1.1b) \quad u(x, t) = 0 \quad \text{on } \partial\Omega \times (0, T],$$

$$(1.1c) \quad u(x, 0) = u_0(x) \quad \text{in } \Omega,$$

where  $\Omega$  is a bounded, convex polygonal domain in  $\mathbb{R}^d$  ( $d \geq 1$ ) with boundary  $\partial\Omega$ ,  $\kappa_\alpha$  and  $u_0$  are given functions defined on their respective domains. Here,  ${}^C\partial_t^\alpha$  is the Caputo time-fractional derivative defined by: for  $0 < \alpha < 1$ ,

$$(1.2) \quad {}^C\partial_t^\alpha \varphi(t) := \mathcal{I}^{1-\alpha} \varphi'(t) := \int_0^t \omega_{1-\alpha}(t-s) \varphi'(s) ds, \quad \text{with } \omega_{1-\alpha}(t) := \frac{t^{-\alpha}}{\Gamma(1-\alpha)},$$

where  $\varphi'$  denotes the (partial) time derivative of  $\varphi$  and for  $\nu > 0$ ,  $\mathcal{I}^\nu$  is the Riemann–Liouville time-fractional integral operator of order  $\nu$  which reduces to the classical definite integral when  $\nu$  is a positive integer. The diffusivity coefficient  $\kappa_\alpha$  satisfies the positivity property:

$$(1.3) \quad 0 < \kappa_{\min} \leq \kappa_\alpha(x, t) \leq \kappa_{\max} < \infty \quad \text{for } (x, t) \in \overline{\Omega} \times [0, T].$$

Numerical solutions for time fractional diffusion problem (1.1) with constant or time-independent diffusion parameter  $\kappa_\alpha$  have been studied by various authors over the last decade. For finite difference (including alternating direction implicit schemes) and finite element (conforming and nonconforming) schemes, we refer to [2, 3, 4, 5, 6, 10, 13, 19, 20, 22, 23] and related references therein. Discontinuous Galerkin (DG) methods (including local DG and hybridizable DG schemes) were investigated in [16, 14, 18], and in [9, 21] the spectral method was studied. The convergence analyses in most of these studies required the solution  $u$  of problem (1.1) to be sufficiently regular including at  $t = 0$  which is not practically the case.

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Having time dependent variable diffusivity  $\kappa_\alpha$  in the fractional diffusion problem (1.1) is indeed very interesting and also practically important. The numerical solutions of (1.1) were considered by a few authors only. For *one-dimensional* spatial domain  $\Omega$ , a finite difference scheme was proposed and analyzed by Alikhanov [1]. In the error analysis, the continuous solution  $u$  was assumed to be smooth including at  $t = 0$ . In [17], a piecewise linear time-stepping DG method combined with the standard Galerkin finite element scheme in space was investigated. The convergence of the scheme had been proven assuming that  $u$  is sufficiently regular. Consequently, the convergence results in these papers are not valid if the initial data  $u_0$  is not sufficiently regular where some compatibility conditions are also required.

For constant diffusivity  $\kappa_\alpha$ , Jin et al. [5] studied the error analysis of the spatial semidiscrete piecewise linear Galerkin finite element scheme for problem (1.1). Over a quasi-uniform spatial mesh, quasi-optimal convergence order results (but optimal with respect to the regularity of the initial data  $u_0$ ) were proved. The used error analysis (based on semigroup) approach can be extended for the case of space dependent parameter  $\kappa_\alpha$ , however is not feasible when  $\kappa_\alpha$  is a time or a time-space dependent function. Therefore, the optimality of the finite element error estimates with respect to the convergence order and to the solution smoothness expressed through the problem data  $u_0$  is indeed missing, even for constant  $\kappa_\alpha$ . So, obtaining optimal finite element error bounds for the case of time-space dependent diffusivity  $\kappa_\alpha$  is definitely challenging.

The aim of this work is to show optimal error estimates with respect to both the convergence order and the regularity of the initial data  $u_0$  of the semidiscrete Galerkin method for problem (1.1) allowing both smooth and nonsmooth  $u_0$ . For each  $t \in (0, T]$ , by using a novel innovative energy arguments approach, we show optimal convergence results in the spatial  $L^2$ - and  $H^1$ -norms over a (conforming) regular triangulation mesh (need not be quasi-uniform). It is straight forward to extend our error analysis approach to allow for an inhomogenous source term or homogenous Neumann boundary conditions in problem (1.1).

Note, for time independent diffusivity  $\kappa_\alpha$ , problem (1.1) can be rewritten as:

$$(1.4) \quad u'(x, t) - {}^R D^{1-\alpha} \operatorname{div}(\kappa_\alpha(x) \nabla u(x, t)) = 0 \quad \text{for } (x, t) \in \Omega \times (0, T],$$

where  ${}^R D^{1-\alpha} u := \frac{\partial}{\partial t}(\mathcal{I}^\alpha u)$  is the Riemann–Liouville fractional derivative. Recently, Karaa et al. [7] investigated the error analysis of the Galerkin finite element scheme applied to problem (1.4). Using a delicate energy argument, optimal error bounds in  $H^m(\Omega)$ - (for  $m = 0, 1$ ) and quasi-optimal in  $L^\infty(\Omega)$ -norms were derived for cases of smooth and nonsmooth initial data. Unfortunately, extending the considered approach for the case of time dependent diffusivity is not feasible.

Outline of the paper. In Section 2, the required regularity assumptions on the solution  $u$  of problem (1.1) will be given. We also state and derive some technical results that will be used in our error analysis. In Section 3, we introduce our semidiscrete Galerkin scheme for problem (1.1) and recall some error projection results from the existing literature. In Section 4, under certain regularity assumptions on the initial data  $u_0$ , optimal error estimates (with respect to both the convergence order and the regularity of  $u_0$ ) in the  $L^2(\Omega)$ -norm will be proved using novel energy arguments, see Theorem 4.3. On the other hand, in the  $H^1(\Omega)$ -norm, for  $t \in (0, T]$  and when  $u_0 \in \dot{H}^\delta(\Omega)$  (this Sobolev space will be defined in the next section), we show an optimal error bounded by  $Ch t^{\alpha(\delta-2)/2}$  for  $0 \leq \delta \leq 2$  (that is, allowing

both smooth and nonsmooth initial data),  $h$  denoting the maximum diameter of the spatial mesh elements, see Subsection 4.1. By further enrichments of the energy arguments approach, optimal  $L^2(\Omega)$ -norm error bounds are achieved in Section 5 for both smooth and nonsmooth  $u_0$ , see Theorem 5.3. For  $t \in (0, T]$  and when  $u_0 \in \dot{H}^\delta(\Omega)$  for  $0 \leq \delta \leq 2$ , an  $O(t^{-\alpha(2-\delta)/2}h^2)$  error estimate is proved. The derived optimal bounds in both  $L^2(\Omega)$ - and  $H^1(\Omega)$ -norms provide remarkable improvements of results obtained by Jin *et al.* in [5, Theorem 3.7]. Therein, for a quasi-uniform mesh and assuming that the parameter  $\kappa_\alpha$  is constant, an  $O(t^{-\alpha(2-\delta)/2}h^{2-m}|\log h|)$  error bound was derived in the  $H^m(\Omega)$ -norm ( $m = 0, 1$ ) when  $u_0 \in \dot{H}^\delta(\Omega)$  with  $\delta = 0, 1, 2$ .

## 2. REGULARITY AND TECHNICAL RESULTS

It is known that the solution  $u$  of problem (1.1) has singularity near  $t = 0$ , even for smooth given data. In our error analysis, we assume that for  $0 \leq p \leq q \leq 2$ ,

$$(2.1) \quad \|u(t)\|_q + t\|u'(t)\|_q \leq Ct^{\alpha(p-q)/2}\|u_0\|_p,$$

where  $\|\cdot\|_r$  denotes the norm on the Hilbert space  $\dot{H}^r(\Omega) \subset L^2(\Omega)$  defined by

$$\|v\|_r^2 = \|\mathcal{L}^{r/2}v\|^2 = \sum_{j=1}^{\infty} \lambda_j^r (v, \phi_j)^2, \quad \text{with } \mathcal{L}v := -\operatorname{div}(\kappa_\alpha \nabla v),$$

where  $\{\lambda_j\}_{j=1}^{\infty}$  (with  $0 < \lambda_1 < \lambda_2 < \dots$ ) are the eigenvalues of the operator  $\mathcal{L}$  (subject homogeneous Dirichlet boundary conditions) and  $\{\phi_j\}_{j=1}^{\infty}$  are the associated orthonormal eigenfunctions. In the above definition,  $(\cdot, \cdot)$  denotes the  $L^2(\Omega)$ -norm and  $\|\cdot\| := \|\cdot\|_0$  is the associated norm. Note,  $\dot{H}^r(\Omega) = H^r(\Omega)$  for  $0 \leq r < 1/2$ , however, for a convex polygonal domain  $\Omega$ ,  $\dot{H}^r(\Omega) = \{w \in H^r(\Omega) : w = 0 \text{ on } \partial\Omega\}$  when  $1/2 < r < 5/2$ , where  $H^r(\Omega)$  (with  $H^0(\Omega) = L^2(\Omega)$ ) is the standard Sobolev space.

Indeed, for time independent function  $\kappa_\alpha$ , the above regularity assumption holds assuming that the domain  $\Omega$  is convex, see Theorems 4.1 and 4.2 in [12]. We conjecture that the same is true for a sufficiently regular time dependent  $\kappa_\alpha$ .

Next, we state some properties of the fractional integral operators  $\mathcal{I}^\alpha$ , and derive some technical results that will be used later. By [15, Lemma 3.1(ii)], it follows that for piecewise time continuous functions  $\varphi : [0, T] \rightarrow L^2(\Omega)$ ,

$$(2.2) \quad \int_0^T (\mathcal{I}^\alpha \varphi, \varphi) dt \geq \cos(\alpha\pi/2) \int_0^T \|\mathcal{I}^{\alpha/2} \varphi\|^2 dt \geq 0 \text{ for } 0 < \alpha < 1.$$

Furthermore, by [15, Lemma 3.1(iii)] and the inequality  $\cos(\alpha\pi/2) \geq 1 - \alpha$ , we obtain the following continuity property of  $\mathcal{I}^\alpha$ : for suitable functions  $\varphi$  and  $\psi$ ,

$$(2.3) \quad \int_0^t (\mathcal{I}^\alpha \varphi, \psi) ds \leq \epsilon \int_0^t (\mathcal{I}^{1-\alpha} \varphi, \varphi) ds + \frac{1}{4\epsilon(1-\alpha)} \int_0^t (\mathcal{I}^{1-\alpha} \psi, \psi) ds, \quad \text{for } \epsilon > 0.$$

In our convergence analysis, we also make use of the following inequality (see [8, Lemma 4] for the proof):

$$(2.4) \quad \|\varphi(t)\|^2 \leq \frac{t^\alpha}{\alpha^2} \int_0^t (\mathcal{I}^{1-\alpha} \varphi', \varphi') ds, \quad \text{for } t > 0.$$

Based on the generalized Leibniz formula and the relation between Riemann–Liouville and Caputo fractional derivatives, we show the identity in the next lemma. For convenience, we use the notations:

$$v_i(t) := t^i v(t), \quad \text{for } i = 1, 2.$$

**Lemma 2.1.** *Let  $0 < \alpha < 1$ . The following holds: for  $0 \leq t \leq T$ ,*

$$t^2 \mathcal{I}^\alpha v'(t) = \mathcal{I}^\alpha v_2'(t) + 2(\alpha - 1) \mathcal{I}^\alpha v_1(t) + \alpha(\alpha - 1) \mathcal{I}^{1+\alpha} v(t) - t^2 \omega_\alpha(t) v(0).$$

*Proof.* Since  $\mathcal{I}^\alpha v'(t) = (\mathcal{I}^\alpha v(t))' - \omega_\alpha(t) v(0)$ , the use of the fractional Leibniz formula  $t(\mathcal{I}^\alpha v(t))' = (\mathcal{I}^\alpha v_1(t))' + (\alpha - 1) \mathcal{I}^\alpha v(t)$  and the equality  $(\mathcal{I}^\alpha v_1(t))' = \mathcal{I}^\alpha v_1'(t)$  yield the following identity:

$$(2.5) \quad t \mathcal{I}^\alpha v'(t) = \mathcal{I}^\alpha v_1'(t) + (\alpha - 1) \mathcal{I}^\alpha v(t) - t \omega_\alpha(t) v(0).$$

Now, multiplying both side of the above identity by  $t$  and applying the identity:  $t \mathcal{I}^\alpha \phi(t) = \mathcal{I}^\alpha \phi_1(t) + \alpha \mathcal{I}^{1+\alpha} \phi(t)$  (see [7, Lemma 4.1 (b)] for the proof) twice,

$$\begin{aligned} t^2 \mathcal{I}^\alpha v'(t) &= t \mathcal{I}^\alpha v_1'(t) + (\alpha - 1) t \mathcal{I}^\alpha v(t) - t^2 \omega_\alpha(t) v(0) \\ &= [\mathcal{I}^\alpha (v_1')_1(t) + \alpha \mathcal{I}^{1+\alpha} v_1'(t)] + (\alpha - 1) [\mathcal{I}^\alpha v_1(t) + \alpha \mathcal{I}^{1+\alpha} v(t)] - t^2 \omega_\alpha(t) v(0). \end{aligned}$$

Since  $(v_1')_1(t) = t v_1'(t) = v_2'(t) - v_1(t)$  and  $\mathcal{I}^{1+\alpha} v_1'(t) = \mathcal{I}^\alpha v_1(t)$ , the desired identity follows after simple simplifications.  $\square$

For the rest of the paper,  $C$  is a generic constant that may depend on  $\alpha$ ,  $T$ , and the norms of  $\kappa_\alpha$ ,  $\kappa'_\alpha$  and  $\kappa''_\alpha$ , but is independent of the spatial mesh size element  $h$ .

**Lemma 2.2.** *Let  $g \geq 0$  be a nondecreasing function of  $t$ .*

(i) *If*

$$(2.6) \quad \int_0^t (\mathcal{I}^{1-\alpha} v, v) ds + 2 \int_0^t (\mathcal{I}(\kappa_\alpha w), w) ds \leq g(t), \quad \text{for } t > 0,$$

*for suitable functions  $v$  and  $w$ , then for  $\kappa'_\alpha \in L^\infty((0, T), L^\infty(\Omega))$ , we have*

$$\int_0^t (\mathcal{I}^{1-\alpha} v, v) ds + \|\mathcal{I} w(t)\|^2 \leq C g(t).$$

(ii) *If*

$$(2.7) \quad \int_0^t (\mathcal{I}^{2-\alpha} v, \mathcal{I} v) ds + 2 \int_0^t (\mathcal{I}^2(\kappa_\alpha w), \mathcal{I} w) ds \leq g(t) \quad \text{for } t > 0,$$

*for suitable functions  $v$  and  $w$ , then for  $\kappa'_\alpha, \kappa''_\alpha \in L^\infty((0, T), L^\infty(\Omega))$ , we have*

$$\int_0^t (\mathcal{I}^{2-\alpha} v, \mathcal{I} v) ds + \|\mathcal{I}^2 w(t)\|^2 \leq C g(t).$$

*Proof.* Let  $w_I(t) := \mathcal{I} w(t) = \int_0^t w(s) ds$ . Since  $\mathcal{I}(\kappa_\alpha w) = \kappa_\alpha w_I - \mathcal{I}(\kappa'_\alpha w_I)$ , an integration by parts yields

$$\begin{aligned} 2 \int_0^t (\mathcal{I}(\kappa_\alpha w), w) ds &= \int_0^t (\kappa_\alpha, (w_I^2)') ds - 2 \int_0^t (\mathcal{I}(\kappa'_\alpha w_I), w_I') ds \\ &= (\kappa_\alpha(t), w_I^2(t)) - \int_0^t (\kappa'_\alpha, w_I^2) ds - 2(\mathcal{I}(\kappa'_\alpha w_I)(t), w_I(t)) + 2 \int_0^t (\kappa'_\alpha, w_I^2) ds \\ &= (\kappa_\alpha(t), w_I^2(t)) - 2(\mathcal{I}(\kappa'_\alpha w_I)(t), w_I(t)) + \int_0^t (\kappa'_\alpha, w_I^2) ds. \end{aligned}$$

Therefore, by inserting this in (2.6), then using the positivity assumption on the diffusion coefficient  $\kappa_\alpha$ , (1.3), and the Cauchy-Schwarz inequality, we conclude that

$$\begin{aligned} \int_0^t (\mathcal{I}^{1-\alpha} v, v) ds + \|w_I(t)\|^2 &\leq Cg(t) + C \int_0^t \|w_I\| ds \|w_I(t)\| + C \int_0^t \|w_I\|^2 ds \\ &\leq Cg(t) + \frac{1}{2} \|w_I(t)\|^2 + C \int_0^t \|w_I\|^2 ds. \end{aligned}$$

Thus,

$$\int_0^t (\mathcal{I}^{1-\alpha} v, v) ds + \|w_I(t)\|^2 \leq Cg(t) + C \int_0^t \|w_I\|^2 ds.$$

Since  $\int_0^t (\mathcal{I}^{1-\alpha} v, v) ds \geq 0$  by the positivity property in (2.2), an application of the continuous version of Gronwall's inequality yields the first desired result.

To show (ii), we let  $w_{II} := \mathcal{I}^2 v$ . Since  $\mathcal{I}(\kappa_\alpha w_{II}'') = \kappa_\alpha w_{II}' - \mathcal{I}(\kappa_\alpha' w_{II}')$ ,

$$\begin{aligned} \mathcal{I}^2(\kappa_\alpha w_{II}'')(s) &= \mathcal{I}(\kappa_\alpha w_{II}')(s) - \mathcal{I}^2(\kappa_\alpha' w_{II}')(s) \\ &= \kappa_\alpha(s) w_{II}(s) - \mathcal{I}(\kappa_\alpha' w_{II})(s) - \mathcal{I}^2(\kappa_\alpha' w_{II}')(s) \\ &= \kappa_\alpha(s) w_{II}(s) - 2\mathcal{I}(\kappa_\alpha' w_{II})(s) + \mathcal{I}^2(\kappa_\alpha'' w_{II})(s). \end{aligned}$$

Thus, an integration by parts yields

$$\begin{aligned} 2 \int_0^t (\mathcal{I}^2(\kappa_\alpha w), \mathcal{I} w) ds &= 2 \int_0^t (\mathcal{I}^2(\kappa_\alpha w_{II}''), w_{II}') ds \\ &= \int_0^t (\kappa_\alpha, (w_{II}^2)') ds - 2 \int_0^t (2\mathcal{I}(\kappa_\alpha' w_{II}) - \mathcal{I}^2(\kappa_\alpha'' w_{II}), w_{II}') ds \\ &= (\kappa_\alpha(t), w_{II}^2(t)) - \int_0^t (\kappa_\alpha', w_{II}^2) ds \\ &\quad - 2(2\mathcal{I}(\kappa_\alpha' w_{II})(t) - \mathcal{I}^2(\kappa_\alpha'' w_{II})(t), w_{II}(t)) + 2 \int_0^t (2\kappa_\alpha' w_{II} - \mathcal{I}(\kappa_\alpha'' w_{II}), w_{II}) ds \\ &= (\kappa_\alpha(t), w_{II}^2(t)) + 3 \int_0^t (\kappa_\alpha', w_{II}^2) ds \\ &\quad - 2(2\mathcal{I}(\kappa_\alpha' w_{II})(t) - \mathcal{I}^2(\kappa_\alpha'' w_{II})(t), w_{II}(t)) - 2 \int_0^t (\mathcal{I}(\kappa_\alpha'' w_{II}), w_{II}) ds. \end{aligned}$$

Now, by proceeding as in the proof of (i), we obtain the second desired result.  $\square$

### 3. FINITE ELEMENT DISCRETIZATION

This section focuses on the spatial semidiscrete Galerkin finite element scheme for the time fractional diffusion problem (1.1). Let  $\mathcal{T}_h$  be a family of shape-regular triangulations (made of simplexes  $K$ ) of the domain  $\bar{\Omega}$  and let  $h = \max_{K \in \mathcal{T}_h} (\text{diam} K)$ , where  $h_K$  denotes the diameter of the element  $K$ . Let  $S_h \in H_0^1(\Omega)$  denote the usual space of continuous, piecewise-linear functions on  $\mathcal{T}_h$  that vanish on  $\partial\Omega$ .

The weak formulation for problem (1.1) is to find  $u : (0, T] \rightarrow H_0^1(\Omega)$  such that

$$(3.1) \quad (\mathcal{C}\partial_t^\alpha u, v) + A(u, v) = 0 \quad \forall v \in H_0^1(\Omega)$$

with given  $u(0) = u_0$ . Here  $A(\cdot, \cdot)$  is the bilinear form associated with the elliptic operator  $\mathcal{L}$ , i.e.,  $A(v, w) = (\kappa_\alpha \nabla v, \nabla w)$ , which is symmetric positive definite on the Sobolev space  $H_0^1(\Omega)$ .

Now, the semidiscrete scheme for (1.1) is to seek  $u_h : (0, T] \rightarrow S_h$  such that

$$(3.2) \quad ({}^C\partial_t^\alpha u_h, \chi) + A(u_h, \chi) = 0 \quad \forall \chi \in S_h,$$

with given  $u_h(0) := u_{h0} = P_h u_0$ , where  $P_h : L^2(\Omega) \rightarrow S_h$  denotes the  $L^2$ -projection defined by  $(P_h v - v, \chi) = 0$  for all  $\chi \in S_h$ . Indeed, for initial data  $u_0 \in \dot{H}^1(\Omega)$ , one may choose instead  $u_h(0) = R_h u_0$ , where  $R_h : H_0^1(\Omega) \rightarrow S_h$  is the Ritz projection defined by the following relation:  $A(R_h v - v, \chi) = 0$  for all  $\chi \in S_h$ .

For the error analysis, we use the following decomposition:

$$(3.3) \quad e := u - u_h = (u - R_h u) - (u_h - R_h u) =: \rho - \theta,$$

For  $t \in (0, T]$ , from the projection error estimates [11, (3.2) and (3.3)],  $\|\rho(t)\| + h\|\rho(t)\|_1 \leq Ch^m \|u(t)\|_m$  and  $\|\rho'(t)\| + h\|\rho'(t)\|_1 \leq Ch^m [\|u(t)\|_m + \|u'(t)\|_m]$  for  $m = 1, 2$ . Hence, by using the regularity property in (2.1), we observe: for  $m = 1, 2$ ,

$$(3.4) \quad \|\rho(t)\| + h\|\rho(t)\|_1 \leq Ch^m t^{\alpha(\delta-m)/2} \|u_0\|_\delta, \quad \text{for } 0 \leq \delta \leq m.$$

and

$$(3.5) \quad t\|\rho'(t)\| + h t\|\rho'(t)\|_1 \leq Ch^m t^{\alpha(\delta-m)/2} \|u_0\|_\delta, \quad \text{for } 0 \leq \delta \leq m.$$

Therefore, for later use, we have

$$(3.6) \quad \begin{aligned} \|\mathcal{I}^{1-\alpha} \rho(t)\| + \|\mathcal{I}^{1-\alpha} \rho'_1(t)\| &\leq C \int_0^t (t-s)^{-\alpha} [\|\rho(s)\| + s\|\rho'(s)\|] ds \\ &\leq Ch^m \int_0^t (t-s)^{-\alpha} s^{\alpha(\delta-m)/2} ds \|u_0\|_\delta \\ &= Ch^m t^{1-\alpha+\alpha(\delta-m)/2} \|u_0\|_\delta, \quad \text{for } 0 \leq \delta \leq m, \text{ with } m = 1, 2. \end{aligned}$$

In a similar fashion, for  $t \in (0, T]$ , we have

$$(3.7) \quad \begin{aligned} \|\mathcal{I}^{1-\alpha} \rho'_2(t)\| + \|\mathcal{I}^{1-\alpha} \rho_1(t)\| &\leq C \int_0^t (t-s)^{-\alpha} [s\|\rho(s)\| + s^2\|\rho'(s)\|] ds \\ &\leq Ch^2 \int_0^t (t-s)^{-\alpha} s^{1+\alpha(\delta-2)/2} ds \|u_0\|_\delta \\ &\leq Ch^2 t^{2-\alpha+\alpha(\delta-2)/2} \|u_0\|_\delta, \quad \text{for } 0 \leq \delta \leq 2. \end{aligned}$$

Via an energy argument approach, we estimate  $\theta$  (and consequently the finite element error) in the next section.

#### 4. ERROR ESTIMATES

This section is devoted to derive optimal error bounds from the Galerkin approximation in both  $L^2(\Omega)$ - and  $H^1(\Omega)$ -norms, assuming that the initial data  $u_0$  satisfies some regularity assumptions for the  $L^2(\Omega)$ -norm error. The main task is to estimate  $\theta$  in (3.3). To do so, we need the bound in the next lemma.

**Lemma 4.1.** *For  $0 < t \leq T$ , we have*

$$\int_0^t (\mathcal{I}^{1-\alpha} \theta, \theta) ds + \|\mathcal{I}(\nabla \theta)(t)\|^2 \leq C \int_0^t |(\mathcal{I}^{1-\alpha} \rho, \rho)| ds.$$

*Proof.* From (3.1) and (3.2), the error decomposition  $e = \rho - \theta$  in (3.3), and the property of the Ritz projection, we obtain

$$(4.1) \quad (\mathcal{I}^{1-\alpha}\theta', \chi) + A(\theta, \chi) = (\mathcal{I}^{1-\alpha}\rho', \chi) \quad \forall \chi \in S_h.$$

We integrate in time and use the identity  $\mathcal{I}^{2-\alpha}v'(t) = \mathcal{I}^{1-\alpha}v(t) - \omega_{2-\alpha}(t)v(0)$ ,

$$(4.2) \quad (\mathcal{I}^{1-\alpha}\theta, \chi) + (\mathcal{I}(\kappa_\alpha \nabla \theta), \nabla \chi) = (\mathcal{I}^{1-\alpha}\rho - \omega_{2-\alpha}(t)e(0), \chi) \quad \forall \chi \in S_h.$$

Since  $(e(0), \chi) = (u_0 - P_h u_0, \chi) = 0$ ,

$$(4.3) \quad (\mathcal{I}^{1-\alpha}\theta, \chi) + (\mathcal{I}(\kappa_\alpha \nabla \theta), \nabla \chi) = (\mathcal{I}^{1-\alpha}\rho, \chi) \quad \forall \chi \in S_h.$$

Choose  $\chi = \theta$  and integrate again in time, we find that

$$\int_0^t (\mathcal{I}^{1-\alpha}\theta, \theta) ds + \int_0^t (\mathcal{I}(\kappa_\alpha \nabla \theta), \nabla \theta) ds = \int_0^t (\mathcal{I}^{1-\alpha}\rho, \theta) ds.$$

By the continuity property of the operator  $\mathcal{I}^{1-\alpha}$  in (2.3) with  $\epsilon = 1/2$ , we have

$$\int_0^t (\mathcal{I}^{1-\alpha}\rho, \theta) ds \leq \frac{1}{2} \int_0^t (\mathcal{I}^{1-\alpha}\theta, \theta) ds + C \int_0^t (\mathcal{I}^{1-\alpha}\rho, \rho) ds,$$

and thus,

$$\int_0^t (\mathcal{I}^{1-\alpha}\theta, \theta) ds + 2 \int_0^t (\mathcal{I}(\kappa_\alpha \nabla \theta), \nabla \theta) ds \leq C \int_0^t |(\mathcal{I}^{1-\alpha}\rho, \rho)| ds.$$

Therefore, an application of Lemma 2.2 (i) yields the desired bound.  $\square$

In the next lemma, we derive an upper bound of  $\theta$  in the spatial  $L^2$ - and  $H^1$ -norms. These bounds may not lead to an optimal convergence rate in the  $L^2(\Omega)$ -norm for nonsmooth  $u_0$ , see Theorem 4.3. To overcome this issue, more delicate energy arguments will be proposed in the next section.

**Lemma 4.2.** *For  $0 \leq t \leq T$ , the following estimate holds*

$$\|\theta(t)\|^2 + t^\alpha \|\nabla \theta(t)\|^2 \leq C t^{\alpha-2} \int_0^t \left[ \|\mathcal{I}^{1-\alpha}\rho\| \|\rho\| + \|\mathcal{I}^{1-\alpha}\rho'_1\| \|\rho'_1\| \right] ds.$$

*Proof.* Multiplying both side of (4.1) by  $t$ , gives

$$(t\mathcal{I}^{1-\alpha}\theta', \chi) + A(\theta_1, \chi) = (t\mathcal{I}^{1-\alpha}\rho', \chi).$$

Hence, by the identity in (2.5) and the equality  $(e(0), \chi) = 0$ , we obtain

$$(4.4) \quad (\mathcal{I}^{1-\alpha}\theta'_1 - \alpha\mathcal{I}^{1-\alpha}\theta, \chi) + A(\theta_1, \chi) = (\mathcal{I}^{1-\alpha}\rho'_1 - \alpha\mathcal{I}^{1-\alpha}\rho, \chi).$$

Choosing  $\chi = \theta'_1$ , then integrating in time and rearranging the terms yield

$$\int_0^t [(\mathcal{I}^{1-\alpha}\theta'_1, \theta'_1) + A(\theta_1, \theta'_1)] ds = \int_0^t [(\mathcal{I}^{1-\alpha}\rho'_1, \theta'_1) - \alpha(\mathcal{I}^{1-\alpha}\rho, \theta'_1) + \alpha(\mathcal{I}^{1-\alpha}\theta, \theta'_1)] ds.$$

By applying the continuity property of  $\mathcal{I}^{1-\alpha}$  in (2.3) (with  $\epsilon = 1/4$ ), the right-hand side in the above equation is

$$\leq \frac{3}{4} \int_0^t [(\mathcal{I}^{1-\alpha}\theta'_1, \theta'_1) ds + C \int_0^t [(\mathcal{I}^{1-\alpha}\rho'_1, \rho'_1) + (\mathcal{I}^{1-\alpha}\rho, \rho) + (\mathcal{I}^{1-\alpha}\theta, \theta)] ds.$$

On the other hand, an integration by parts follows by using the positivity assumption of  $\kappa_\alpha$  in (1.3), yielding

$$\begin{aligned}
 2 \int_0^t A(\theta_1, \theta'_1) ds &= \int_0^t (\kappa_\alpha, ((\nabla \theta_1)^2)') ds \\
 (4.5) \qquad \qquad \qquad &= (\kappa_\alpha(t), (\nabla \theta_1)^2(t)) - \int_0^t (\kappa'_\alpha, (\nabla \theta_1)^2) ds \\
 &\geq \kappa_{\min} \|\nabla \theta_1(t)\|^2 - \int_0^t (\kappa'_\alpha, (\nabla \theta_1)^2) ds,
 \end{aligned}$$

Therefore, after combining the above three equations, we conclude that

$$\begin{aligned}
 &\int_0^t (\mathcal{I}^{1-\alpha} \theta'_1, \theta'_1) ds + \|\nabla \theta_1(t)\|^2 \\
 &\leq C \int_0^t [(\mathcal{I}^{1-\alpha} \rho'_1, \rho'_1) + (\mathcal{I}^{1-\alpha} \rho, \rho) + (\mathcal{I}^{1-\alpha} \theta, \theta)] ds + C \int_0^t \|\nabla \theta_1\|^2 ds.
 \end{aligned}$$

Thus, an application of the Gronwall's inequality gives

$$\int_0^t (\mathcal{I}^{1-\alpha} \theta'_1, \theta'_1) ds + \|\nabla \theta_1(t)\|^2 \leq C \int_0^t [(\mathcal{I}^{1-\alpha} \rho'_1, \rho'_1) + (\mathcal{I}^{1-\alpha} \rho, \rho) + (\mathcal{I}^{1-\alpha} \theta, \theta)] ds.$$

Finally, using (2.4) for finding a lower bound of the first term in the above equation, and Lemma 4.1 for estimating the last term, and the identity  $\theta(t) = t^{-1} \theta_1(t)$  will complete the proof.  $\square$

In the next theorem, for each  $t \in (0, T]$ , we show that the spatial  $L^2$ -norm error is bounded by  $Ch^2 t^{\alpha(\delta-2)/2} \|u_0\|_\delta$  with  $\delta \in (3 - 2/\alpha, 2] \cap [0, 2]$ . Thus, for  $\alpha > 2/3$ , this bound is not valid when  $u_0 \in \dot{H}^\delta(\Omega)$  with  $0 \leq \delta \leq 3 - 2/\alpha$ . This regularity issue will be resolved by showing a sharper upper bound of the term  $\theta$  via more delicate energy arguments, see Theorem 5.3.

**Theorem 4.3.** *Let  $u$  and  $u_h$  be the solutions of (1.1) and (3.2), respectively, with  $u_{h0} = P_h u_0$ . Let  $u_0 \in \dot{H}^\delta(\Omega)$  and  $\kappa'_\alpha \in L^\infty((0, T), L^\infty(\Omega))$ . Then, for  $t \in (0, T]$ ,*

$$\|(u - u_h)(t)\| \leq Ch^2 t^{\alpha(\delta-2)/2} \|u_0\|_\delta, \quad \text{for } \delta \in (3 - 2/\alpha, 2] \cap [0, 2].$$

*Proof.* Using the estimates in (3.4), (3.5), and (3.6) with  $m = 2$ , we find after integration that for  $t \in (0, T]$ ,

$$\begin{aligned}
 \int_0^t [\|\mathcal{I}^{1-\alpha} \rho\| \|\rho\| + \|\mathcal{I}^{1-\alpha} \rho'_1\| \|\rho'_1\|] ds &\leq Ch^4 \int_0^t s^{\alpha(\delta-3)+1} ds \|u_0\|_\delta^2 \\
 &= Ch^4 t^{2+\alpha(\delta-3)} \|u_0\|_\delta^2 \text{ for } \delta \in (3 - 2/\alpha, 2] \cap [0, 2].
 \end{aligned}$$

Thus, by using Lemma 4.2, we find that

$$(4.6) \qquad \|\theta(t)\|^2 \leq Ch^4 t^{\alpha(\delta-2)} \|u_0\|_\delta^2 \text{ for } \delta \in (3 - 2/\alpha, 2] \cap [0, 2].$$

Therefore, the desired bound follows from the decomposition  $u - u_h = \rho - \theta$ , the estimate of  $\rho$  in (3.4) for  $m = 2$ , and the above bound.  $\square$



**4.1. Convergence in the spatial  $H^1$ -norm.** When  $u_0 \in \dot{H}^\delta(\Omega)$  with  $0 \leq \delta \leq 1$ , we use (3.4), (3.5) and (3.6) but with  $m = 1$ , and get

$$\begin{aligned} \int_0^t \left[ \|\mathcal{I}^{1-\alpha} \rho\| \|\rho\| + \|\mathcal{I}^{1-\alpha} \rho'_1\| \|\rho'_1\| \right] ds &\leq C h^2 \|u_0\|_\delta^2 \int_0^t s^{1-\alpha+\alpha(\delta-1)} ds \\ &\leq C h^2 t^{2-2\alpha+\alpha\delta} \|u_0\|_\delta^2, \quad \text{for } 0 \leq \delta \leq 1. \end{aligned}$$

Hence, by Lemma 4.2,

$$\|\nabla \theta(t)\|^2 \leq C h^2 t^{\alpha(\delta-2)} \|u_0\|_\delta^2, \quad \text{for } 0 \leq \delta \leq 1.$$

Therefore, from the decomposition  $u - u_h = \rho - \theta$ , the above estimate, and (3.4) with  $m = 1$ , we reach the following  $H^1(\Omega)$ -norm optimal error bound (with respect to both the convergence order and the regularity of the initial data):

$$\|\nabla(u - u_h)(t)\| \leq C h t^{\alpha(\delta-2)/2} \|u_0\|_\delta, \quad \text{for } 0 \leq \delta \leq 1.$$

However, for  $u_0 \in \dot{H}^\delta(\Omega)$  with  $1 < \delta \leq 2$ , we proceed as in Theorem 4.3 and obtain

$$\int_0^t \left[ \|\mathcal{I}^{1-\alpha} \rho\| \|\rho\| + \|\mathcal{I}^{1-\alpha} \rho'_1\| \|\rho'_1\| \right] ds \leq C h^4 t^{2-3\alpha+\alpha\delta} \|u_0\|_\delta^2, \quad \text{for } 1 < \delta \leq 2.$$

Once again, by Lemma 4.2,

$$\|\nabla \theta(t)\|^2 \leq C h^2 t^{\alpha(\delta-2)} (h^2 t^{-\alpha}) \|u_0\|_\delta^2, \quad \text{for } 1 < \delta \leq 2.$$

Thus, following the above arguments and using (3.4) with  $m = 2$ , we find that

$$\|\nabla(u - u_h)(t)\| \leq C h t^{\alpha(\delta-2)/2} \max\{h t^{-\alpha/2}, 1\} \|u_0\|_\delta, \quad \text{for } 1 < \delta \leq 2.$$

This error bound is optimal provided that  $h^2 \leq t^\alpha$ . Indeed, by assuming that the spatial mesh is quasi-uniform, this optimality can also be preserved even if  $h^2 > t^\alpha$ . To see this, we apply the inverse inequality and use the achieved estimate in (4.6),

$$(4.7) \quad \|\nabla \theta(t)\| \leq C h^{-1} \|\theta(t)\| \leq C h^2 t^{\alpha(\delta-2)/2} \|u_0\|_\delta, \quad \text{for } 1 < \delta \leq 2.$$

Hence, for  $t \in (0, T]$ , we have

$$\|\nabla(u - u_h)(t)\| \leq C h t^{\alpha(\delta-2)/2} \|u_0\|_\delta, \quad \text{for } 1 < \delta \leq 2.$$

## 5. IMPROVED ERROR ESTIMATES

The obtained error results in Theorem 4.3 will be improved in this section. For  $t \in (0, T]$  and for  $u_0 \in \dot{H}^\delta(\Omega)$ , we show an  $O(h^2 t^{\alpha(\delta-2)/2})$  error bound in  $L^2(\Omega)$ -norm for  $0 \leq \delta \leq 2$ , which is optimal for both cases smooth and nonsmooth initial data  $u_0$ . The estimate of  $\theta_1$  in the lemma below (which is a stronger version of Lemma 4.1) plays a crucial role in achieving our goal.

**Lemma 5.1.** *For  $0 \leq t \leq T$ , we have*

$$\int_0^t (\mathcal{I}^{1-\alpha} \theta_1, \theta_1) + \|\mathcal{I}(\nabla \theta_1)(t)\|^2 \leq C \int_0^t [|\langle \mathcal{I}^{1-\alpha} \rho_1, \rho_1 \rangle| + |\langle \mathcal{I}^{2-\alpha} \rho, \mathcal{I} \rho \rangle|] ds.$$

*Proof.* Integrating (4.4) in time and rearranging the terms to get

$$(\mathcal{I}^{1-\alpha} \theta_1, \chi) + (\mathcal{I}(\kappa_\alpha \nabla \theta_1), \nabla \chi) = (\mathcal{I}^{1-\alpha} \rho_1 - \alpha \mathcal{I}^{1-\alpha}(\mathcal{I} \rho) + \alpha \mathcal{I}^{1-\alpha}(\mathcal{I} \theta), \chi),$$

for all  $\chi \in S_h$ . Choosing  $\chi = \theta_1$ , and then integrating again in time and using the continuity property in (2.3) (with  $\epsilon = \frac{1}{4}$ ) for the three terms on the right-hand side, we observe that

$$(5.1) \quad \begin{aligned} & \int_0^t [(\mathcal{I}^{1-\alpha}\theta_1, \theta_1) + (\mathcal{I}(\kappa_\alpha \nabla \theta_1), \nabla \theta_1)] ds \\ &= C \int_0^t [(\mathcal{I}^{1-\alpha}\rho_1, \rho_1) + (\mathcal{I}^{1-\alpha}(\mathcal{I}\rho), \mathcal{I}\rho) + (\mathcal{I}^{1-\alpha}(\mathcal{I}\theta), \mathcal{I}\theta)] ds. \end{aligned}$$

To estimate the last term on the right-hand side of (5.1), we integrate (4.3),

$$(5.2) \quad (\mathcal{I}^{1-\alpha}(\mathcal{I}\theta), \chi) + (\mathcal{I}^2(\kappa_\alpha \nabla \theta), \nabla \chi) = (\mathcal{I}^{1-\alpha}(\mathcal{I}\rho), \chi) \quad \forall \chi \in S_h.$$

Setting  $\chi = \mathcal{I}\theta$  and then, integrating over the time interval  $(0, t)$  and applying the continuity property of  $\mathcal{I}^{1-\alpha}$  (with  $\epsilon = \frac{1}{2}$ ), we find that

$$\begin{aligned} & \int_0^t (\mathcal{I}^{1-\alpha}(\mathcal{I}\theta), \mathcal{I}\theta) ds + \int_0^t (\mathcal{I}^2(\kappa_\alpha \nabla \theta), \mathcal{I}(\nabla \theta)) ds = \int_0^t (\mathcal{I}^{1-\alpha}(\mathcal{I}\rho), \mathcal{I}\theta) ds \\ & \leq \frac{1}{2} \int_0^t (\mathcal{I}^{1-\alpha}(\mathcal{I}\theta), \mathcal{I}\theta) ds + C \int_0^t (\mathcal{I}^{1-\alpha}(\mathcal{I}\rho), \mathcal{I}\rho) ds. \end{aligned}$$

After simplifications, an application of Lemma 2.2 (ii) gives

$$(5.3) \quad \int_0^t (\mathcal{I}^{2-\alpha}\theta, \mathcal{I}\theta) ds \leq C \int_0^t |(\mathcal{I}^{2-\alpha}\rho, \mathcal{I}\rho)| ds.$$

Inserting this bound in (5.1) gives

$$\int_0^t [(\mathcal{I}^{1-\alpha}\theta_1, \theta_1) + (\mathcal{I}(\kappa_\alpha \nabla \theta_1), \nabla \theta_1)] ds \leq C \int_0^t [|\mathcal{I}^{1-\alpha}\rho_1| + |(\mathcal{I}^{2-\alpha}\rho, \mathcal{I}\rho)|] ds.$$

Finally, an application of Lemma 2.2 (i) yields the desired bound.  $\square$

Assuming that  $\kappa'_\alpha, \kappa''_\alpha \in L^\infty((0, T), L^\infty(\Omega))$ , a stronger estimate of  $\theta$  will be derived in the next lemma. This will allow us to show optimal error estimates in the  $L^2(\Omega)$ -norm for both smooth and nonsmooth initial data.

**Lemma 5.2.** *For  $0 \leq t \leq T$ , the following estimate holds*

$$\|\theta(t)\|^2 + t^\alpha \|\nabla \theta(t)\|^2 \leq Ct^{\alpha-4} \int_0^t \left[ \|\mathcal{I}^{1-\alpha}\rho'_2\| \|\rho'_2\| + \|\mathcal{I}^{1-\alpha}\rho_1\| \|\rho_1\| + \|\mathcal{I}^{2-\alpha}\rho\| \|\mathcal{I}\rho\| \right] ds.$$

*Proof.* Multiplying both sides of (4.1) by  $t^2$  gives

$$(t^2 \mathcal{I}^{1-\alpha}\theta', \chi) + A(\theta_2, \chi) = (t^2 \mathcal{I}^{1-\alpha}\rho', \chi) \quad \forall \chi \in S_h.$$

Using the identity in Lemma 2.1 and the fact that  $(e(0), \chi) = 0$  yields

$$(5.4) \quad (\mathcal{I}^{1-\alpha}[\theta'_2 - 2\alpha\theta_1 - \alpha(1-\alpha)\mathcal{I}\theta], \chi) + A(\theta_1, \chi) = (\mathcal{I}^{1-\alpha}\eta, \chi), \quad \forall \chi \in S_h.$$

where

$$(5.5) \quad \eta = \rho'_2 - 2\alpha\rho_1 - \alpha(1-\alpha)\mathcal{I}\rho.$$

Rearranging the terms,

$$(\mathcal{I}^{1-\alpha}\theta'_2, \chi) + A(\theta_2, \chi) = (\mathcal{I}^{1-\alpha}\eta, \chi) + 2\alpha(\mathcal{I}^{1-\alpha}\theta_1, \chi) + \alpha(1-\alpha)(\mathcal{I}^{1-\alpha}(\mathcal{I}\theta), \chi).$$

Setting  $\chi = \theta'_2$ , integrating over the time interval  $(0, t)$ , and then, using (4.5) with  $\theta_2$  in place of  $\theta_1$ , and the continuity property of  $\mathcal{I}^{1-\alpha}$  in (2.3) (for an appropriate choice of  $\epsilon$ ) for each term on the right-hand side, we reach

$$\begin{aligned} \int_0^t (\mathcal{I}^{1-\alpha} \theta'_2, \theta'_2) ds + \|\nabla \theta_2(t)\|^2 &\leq C \int_0^t \|\nabla \theta_2\|^2 ds + \frac{1}{2} \int_0^t (\mathcal{I}^{1-\alpha} \theta'_2, \theta'_2) ds \\ &\quad + C \int_0^t [(\mathcal{I}^{1-\alpha} \eta, \eta) + (\mathcal{I}^{1-\alpha} \theta_1, \theta_1) + (\mathcal{I}^{2-\alpha} \theta, \mathcal{I} \theta)] ds. \end{aligned}$$

Simplifying, and then using (5.3) and Lemma 5.1, we obtain

$$\int_0^t (\mathcal{I}^{1-\alpha} \theta'_2, \theta'_2) ds + \|\nabla \theta_2(t)\|^2 \leq C \int_0^t |(\mathcal{I}^{1-\alpha} \eta, \eta)| ds + C \int_0^t \|\nabla \theta_2\|^2 ds.$$

Therefore, applications of the inequality in (2.4) and the Gronwalls inequality yield

$$t^{-\alpha} \|\theta_2(t)\|^2 + \|\nabla \theta_2(t)\|^2 \leq C \int_0^t |(\mathcal{I}^{1-\alpha} \eta, \eta)| ds.$$

The desired result follows immediately after using the fact that  $\theta(t) = t^{-2} \theta_2(t)$ , the definition of  $\eta$  in (5.5) and the Cauchy-Schwarz inequality.  $\square$

In the next theorem, we show that the error from the spatial discretization by the scheme (3.2) is bounded by  $Ch^2 t^{\alpha(\delta-2)/2} \|u_0\|_\delta$  in the  $L^2(\Omega)$ -norm for  $0 \leq \delta \leq 2$ .

**Theorem 5.3.** *Let  $u$  be the solution of the time fractional diffusion problem (1.1) and let  $u_h$  be the finite element solution defined by (3.2), with  $u_{h0} = P_h u_0$ . Assume that  $\kappa'_\alpha, \kappa''_\alpha \in L^\infty((0, T), L^\infty(\Omega))$ . Then, for  $t \in (0, T]$ , we have*

$$\|(u - u_h)(t)\| \leq Ch^2 t^{\alpha(\delta-2)/2} \|u_0\|_\delta \quad \text{for } 0 \leq \delta \leq 2.$$

*Proof.* By using the estimate in (3.7) and the projection error bounds in (3.4)–(3.6) (with  $m = 2$ ) and (3.7), we find that for  $t \in (0, T]$ ,

$$\begin{aligned} \int_0^t \left[ \|\mathcal{I}^{1-\alpha} \rho'_2\| \|\rho'_2\| + \|\mathcal{I}^{1-\alpha} \rho_1\| \|\rho_1\| + \|\mathcal{I}^{2-\alpha} \rho\| \|\mathcal{I} \rho\| \right] ds \\ \leq Ch^4 \int_0^t s^{2-\alpha+\alpha(\delta-2)/2} s^{1+\alpha(\delta-2)/2} ds \|u_0\|_\delta^2 \\ \leq Ch^4 t^{4-\alpha+\alpha(\delta-2)} \|u_0\|_\delta^2, \quad \text{for } 0 \leq \delta \leq 2. \end{aligned}$$

Now, the desired bound follows from the decomposition  $u - u_h = \rho - \theta$ , the estimate of  $\rho$  in (3.4), the estimate of  $\theta$  in Lemma 5.2, and the above bound.  $\square$

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